PATENT
Attorney Docket No.: 020910-000210US

IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

In re application of:

Dan E. Rosenthal

Application No.: 10/053,354

Filed: November 2, 2001

For: METHOD FOR RESIDUAL FORM IN MOLECULAR MODELING

Examiner: Unassigned

Art Unit: 2123

SUPPLEMENTAL INFORMATION DISCLOSURE STATEMENT UNDER 37 CFR §1.97 and §1.98

Assistant Commissioner for Patents
Washington, D.C. 20231

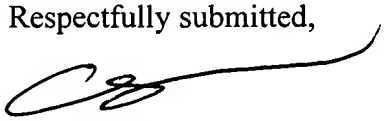
Sir:

The references cited on attached form PTO/SB/08A and PTO/SB/08B are being called to the attention of the Examiner. Copies of the references are enclosed. It is respectfully requested that the cited references be expressly considered during the prosecution of this application, and the references be made of record therein and appear among the "references cited" on any patent to issue therefrom.

As provided for by 37 CFR 1.97(g) and (h), no representation is being made that a search has been conducted or that this statement encompasses all the possible relevant information, and no inference should be made that the information and references cited are, or are considered to be material to patentability because they are in this statement. No inference should be made that the information and references cited are prior art merely because they are in this statement.

Applicant believes that no fee is required for submission of this statement. However, if a fee is required, the Commissioner is authorized to deduct such fee from the undersigned's Deposit Account No. 50-2599. Please deduct any additional fees from, or credit any overpayment to, the above-noted Deposit Account.

Respectfully submitted,



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INFORMATION DISCLOSURE STATEMENT BY APPLICANT

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Sheet 1 of 4

Complete if Known	
Application Number	10/053,354
Filing Date	November 2, 2001
First Named Inventor	Rosenthal, Dan E.
Art Unit	2123
Examiner Name	Unassigned
Attorney Docket Number	020910-000210US

U.S. PATENT DOCUMENTS

Examiner	Cite No.[1]	Document Number: Number Kind Code[2] (*if known*)	Publication Date MM-DD-YYYY	Name of Patentee or Applicant of Cited Document	Pages, Columns, Lines, Where Relevant Passages or Relevant Figures Appear
	AA	US 6,512,997	1/28/2003	Padilla, et al.	
	AB	US 6,253,166	6/26/2001	Whitmore, et al.	
	AC	US 6,185,506	2/6/2001	Cramer, III, et al.	
	AD	US 6,161,080	12/12/2000	Aouni-Ateshian, et al.	
	AE	US 6,150,179	11/21/2000	Went	
	AF	US 6,125,235	9/26/2000	Padilla, et al.	
	AG	US 6,081,766	6/27/2000	Chapman, et al.	
	AH	US 6,014,449	1/11/2000	Jacobs, et al.	
	AI	US 5,799,312	8/25/1998	Rigoutsos	
	AJ	US 5,787,279	7/28/1998	Rigoutsos	
	AK	US 5,777,889	7/7/1998	Mohanty, et al..	
	AL	US 5,752,019	5/12/1998	Rigoutsos, et al.	
	AM	US 5,745,385	4/28/1998	Hinsberg, III, et al.	
	AN	US 5,625,575	4/29/1997	Goyal, et al.	
	AO	US 5,553,004	9/3/1996	Gronbech-Jensen, et al.	
	AP	US 5,307,287	4/26/1994	Cramer, III, et al.	

FOREIGN PATENT DOCUMENTS

Examiner Initials*	Cite No.[1]	Foreign Patent Document: Country Code[3]	Number[4]	Kind Code[5] (*if known*)	Publication Date MM-DD-YYYY	Name of Patentee or Applicant of Cited Document	Pages, Columns, Lines, Where Relevant Passages or Relevant Figures Appear	T[6]
	AQ	WO	02/073334	A2	07-26-1990	Padilla, et al.		☐
	AR	WO	01/67310	A1	12-12-1991	Smith, et al.		☐
	AS	WO	96/24902	A1	04-01-1993	Wertz		☐

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OTHER PRIOR ART -- NON PATENT LITERATURE DOCUMENTS			
Examiner Initials *	Cite No.[1]	Include name of the author (in CAPITAL LETTERS), title of the article (when appropriate), title of the item (book, magazine, journal, serial, symposium, catalog, etc.), date, page(s), volume-issue number(s), publisher, city and/or country where published.	T[2]
	AT	ASCHER, et al., Computer Methods for Ordinary Differential Equations and Differential-Algebraic Equations, 1998, pgs. 3-122 and 231-297, SIAM, Philadelphia, PA.	
	AU	BARAFF, et al., "*Large steps in cloth simulation*", 1998, Computer Graphics Proceedings SIGGRAPH 98 (Orlando, July 19-24) p43.pdf	
	AV	BARTH, et al., "*A separating framework for increasing the timestep in molecular dynamics*" in Computer Simulation of Biomolecular Systems - Theoretical and Experimental Applications, Volume 3, 1997, pgs. 97-121, Kluwer AcademicDordrecht, The Netherlands.	
	AW	BERENDSEN, "*Molecular Dynamics Simulations: The Limits and Beyond*" in Computational Molecular Dynamics: Challenges, Methods, Ideas, 1999, pgs. 3-36, Springer-Verlang, Germany.	
	AX	BISCHOF, et al., ADIFOR 2.0 Users' Guide, 1998, Argonne National Laboratory, University of Chicago, Argonne, IL.	
	AY	BRENAN, et al., Numerical Solution of Initial-Value Problems in Differential-Algebraic Equations, 1989, Chapter 5 (pgs. 115-148), Elsevier Science Publishing Co., New York, NY.	
	AZ	BUTCHER, "*Towards efficient implementation of singly-implicit methods*", 1988, AMC Transactions of Mathematical Software **14**:68-75.	
	BA	BYSTROFF, "*An alternative derivation of the equations of motion in torsion space for a branched linear chain*", 2001, Protein Engineering **14**:825-828.	
	BB	COLEMAN, et al., "*The efficient computation of sparse Jacobian matrices using automatic differentiation*", 1996, Cornell Theory Center Technical Report CTC95TR225.	
	BC	EICHBERGER, et al., "*The benefits of parallel multibody simulation*", 1994, International Journal for Numerical Methods in Engineering, **37**:1557-1572.	
	BD	GOLUB, et al., "*The Differentiation of Pseudo-Inverses and Non-Linear Least Squares Problems Whose Variables Separate*", 1973, SIAM J. Numer Anal. **10**:413.	
	BE	HAIRER, et al., Solving Ordinary Differential Equations II: Stiff and Differential-Algebraic Problems, 2nd ed., 1996, Springer-Verlang, Germany.	
	BF	HE, et al., "*Macromolecular conformational dynamics in torsional angle space*", 1998, Journal of Chemical Physics **108**:271.	
	BG	HOLLARS, et al., SD/FAST User's Manual, Version B.2, 1994, Symbolic Dynamics, California.	

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	BH	IZAGUIRRE, et al., "Longer Time Steps for Molecular Dynamics", 1999, J.Chem.Phys. **110**:9853.	
	BI	KANE, Dynamics, 3rd ed., 1978, Stanford University, Stanford, California.	
	BJ	LEACH, Molecular Modelling Principles and Applications, 2nd ed., 1996, Chapter 6 (pgs. 303-352) Pearson Education Limited, England.	
	BK	MARTINS, et al., "*An automated method for sensitivity analysis using complex variables*", 2000, American Institute of Arenautics and Astronoautics, 2000-0689 p1	
	BL	MOROKUMA, et al., "*Model studies of the structures, reactivities, and reaction mechanisms of metalloenzymes*", 2001, IBM J. Res. & Dev. **45**(3/4):367-395.	
	BM	NORSETT, et al., "*Embedded SDIRK-methods of basic order three*", 1984, BIT **24**:634-646.	
	BN	PONDER, TINKER User's Guide, Version 3.8, October 2000, Washington University, St. Louis, MO.	
	BO	RAPAPORT, The Art of Molecular Dynamics Simulation, 1995, reprinted with corrections 1998, Chapter 3 (pgs. 42-77), Cambridge University Press, United Kingdom.	
	BP	SCHLICK, "*Biomolecular Dynamics at Long Timesteps: Bridging the Timescale Gap Between Simulation and Experimentation*", 1997, Annu. Rev. Biophys. Biomol. Struct., 26:181-222.	
	BQ	SCHLICK, "*Some Failures and Successes of Long-Timestep Approaches to Biomolecular Simulations*" in Computational Molecular Dynamics: Challenges, Methods, Ideas, 1999, pgs. 227-262, Springer-Verlang, Germany.	
	BR	SCHLICK, Molecular Modeling and Simulation - An Interdisciplinary Guide, 2002, Chapter 13 and References, pgs. 419-462 and 561-619, Springer-Verlang, Germany.	
	BS	SHAMPINE, "*Implementation of implicit formulas for the solution of ODEs*", 1980, SIAM J. Sci. Stat. Comput. 1:103-118.	
	BT	VERLET, "*Computer Experiments on Classical Fluids. I. Thermodynamical Properties of Lennard-Jones Molecules*", 1967, Physical Review, **159**(1):98-103.	
	BU	VON SCHWERIN, Multibody System Simulation, 1999, Springer-Verlang, Germany.	

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	BV	WU, et al., "*Constraint dynamics algorithm for simulation of semiflexible macromolecules*", 1998, Journal of Computational Chemistry 19:1555-1566	
	BW	YEN, et al., "*On the numerical solution of constrained multibody dynamic systems*", 1994, University of Minnesota AHPCRC 94-038.	

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